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CENTRAL RESEARCH INSTITUTE FOR PHYSICS

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ABSTRACT

The hyperfine field distribution around Co impurities in iron and the average hyperfine field were measured by Mössbauer and continuous wave nuclear magnetic resonance methods. Analysis of the Mössbauer spectra yielded relative hyperfine field shifts of 4,0 ± 0,6 % and 2,1 ± 0,8 % for the first and second neighbours. The satellites observed in the NMR spectra were shifted by 1,3 ± 0,02 % and 0,18 ± 0,04 % and are interpreted as the contributions of the third and fourth neighbours. The concentration dependence of the average hyperfine field /dH/dc = +190 kOe/ is discussed in the framework of the Campbell-Daniel-Friedel theory.

РЕЗЮМЕ

Мы измеряли методами Мессбауэра и постоянно возбужденного ядерного магнитного резонанса распределение сверхтонких полей вокруг примесей Co в железе и среднее сверхтонкое поле. Анализ мессбауэровских спектров дал на месте первого и второго соседей относительное отклонение сверхтонкого поля в размере 4,0 ± 0,6% и 2,I ± 0,8%. Сателлиты ЯМР с отклонением I,3 ± 0,02% и 0,I8 ± 0,04% мы трактуем в качестве продукта третьего и четвертого соседей. Зависимость концентрации сверхтонкого поля (dн/dc = + I90 коэ) мы интерпретируем на основе теории Кэмпбеля-Даниеля-Фриделя.

KIVONAT

Mössbauer-technikával és folytonos gerjesztésü NMR módszerrel mértük vasban a hiperfinom tér átlagértékét és a Co-szennyezők körüli eloszlását. A Mössbauer-spektrumok elemzéséből az első és második szomszédoknál a hiperfinom tér relativ eltolódására 4,0 ± 0,6 % ill. 2,1 ± 0,8 % adódott. Az NMR spektrumokban megfigyelt szatellitek 1,3 ± 0,02 % ill. 0,18 ± 0,04 % eltolódást mutattak, amit a harmadik és negyedik szomszédok járulékaként értelmeztünk. Az átlagos hiperfinom tér koncentrációfüggését /dH/dc = + 190 kOe/ a Campbell-Daniel-Friedel elmélet keretében tárgyaljuk.

The iron-rich Fe-Co binary alloy system is one of the most investigated ferromagnetic alloys. The hyperfine field distribution around the Co impurities has been measured by a number of authors /for a detailed literature see [1]/. Continuous wave /cwNMR/ and spin echo /SE/ nuclear magnetic resonance experiments show a broadening of the resonance line and a pronounced satellite shifted by $\Delta H/H = 1{,}3$ %. According to Mendis and Anderson [2] and Budnick [3], this satellite corresponds to the third neighbours, but in contrast Rubinstein [1] has suggested that it arises from the first and second neighbours. The contribution of the conduction electron polarization /CEP/ term to the hyperfine field distribution depends closely on these assignments. Comparing the measured shifts with the diffuse neutron scattering /DNS/ data [4], the first assignment implies a large CEP contribution, while Rubinstein's suggestion implies that it is neglibile. The aim of the present paper is to report new cwNMR and Mössbauer /ME/ experiments in an attempt to resolve the above disagreement and also to discuss the concentration dependence of the average hyperfine field in the light of the Campbell-Daniel-Friedel theory.

The cwNMR spectra were measured with a modified Robinson-type oscillator using adiabatic fast passage [2]. The ME experiments were performed with equipment of 1 ‰ linearity operated in a folded mode using a ^{57}Co source diffused in Cr. For the cwNMR investigation Fe-Co alloys containing 0,3; 0,6; 0,72 and 1,41 at% Co were employed, and for the ME experiments alloys with 1,41 and 2,8 at% Co.

The cwNMR spectrum of the 0,72 at% Co alloy is shown in Fig. 1. Two satellites can be seen in the figure, the first at 45,97 Mc/s and the second at 45,46 Mc/s. The second satellite is resolved only at low Co concentrations, and the intensity of the line indicates that it corresponds to the fourth neighbours of the Co impurities. Although it has been suggested [1] that the first satellite should be split by about 75 kc/s due to a difference between the hyperfine fields at the first and the second neighbours, careful examination shows no splitting. The shape of this satellite is similar to that of the central resonance, with a relative intensity corresponding to that of third neighbour contributions.

The Mössbauer spectra exhibit a superposition of 6-line patterns of iron atoms in different environments and resemble a broadened spectrum of pure iron. The average value of the hyperfine field, obtained by computer fit of a 6-line pattern to each of the spectra, yields $dH_{av}/dc = +190 \pm 20$ kOe. The average value of the isomer shift is equal to the isomer shift of pure iron. Attributing the broadening of the spectra to the different environments of the iron atoms, it was assumed that each 6-line pattern consists of Lorentzian curves of equal widths. The hyperfine field was expressed as $H_o + n\Delta H_1 + m\Delta H_2$, where n and m are the numbers of first and second neighbour Co atoms. A similar expression was used for the isomer shift. Decomposition of the spectra by an iteration program yields $\Delta H_1/H = 0{,}040 \pm 0{,}006$ for the first and $\Delta H_2/H = 0{,}021 \pm \pm 0{,}008$ for the second neighbour hyperfine field shifts.[x] The hyperfine field distribution around Co impurities, based on the ME and cwNMR data, is shown in Fig.2. The change of

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x/ Recent ME experiments [5] yield hyperfine field shifts at the first and second neighbours of $0{,}035 \pm 0{,}003$ and $0{,}030 \pm \pm 0{,}006$, in good agreement with our data within the experimental errors.

the average hyperfine field due to one impurity can be computed from the measured shifts, and for low impurity concentrations $dH_{av}/dc = +210 \pm 30$ kOe, which agrees well with the "direct" ME determination. This further supports the validity of the measured hyperfine field distribution.

The hyperfine field receives two main contributions: that from the core polarization H_{CP} and that from the conduction electron polarization H_{CEP}. The former is proportional to the moment localized on the atomic site, the latter to the polarization of the 4s-like band due to interaction with the 3d-like band. The measured hyperfine field distribution thus reflects the perturbation of both the 3d and the 4s-like bands. No attempt has been made yet, as far as we know, to take into account the contributions of the 3d and 4s bands and determine the radial distribution of the perturbation in the case of transitional impurities. Here only the average hyperfine field will be considered in terms of the Campbell-Daniel-Friedel [6] theory.

This theory takes into account the average change of both the CP and CEP terms:

$$\frac{dH_{av}}{dc} = \frac{dH_{CEP}}{dc} + \frac{dH_{CP}}{dc}$$

$$\frac{dH_{CP}}{dc} = h_{CP}\left[\frac{d\mu}{dc} - \left(\mu_i - \mu_h\right)\right] \qquad /1/$$

$$\frac{dH_{CEP}}{dc} = h_{CEP}\left[\frac{d\mu}{dc} - 0{,}4\left(\mu_i - \mu_h\right)\right]$$

where μ is the average magnetic moment of the alloy, μ_i and μ_h are moments of the impurity and the Fe atom, respectively. The parameters in /1/ are $h_{CP} = 50$ kOe/μ_B and $h_{CEP} = 100$ kOe/μ_B.

For comparison with the experimental data the moments evaluated from the NDS experiments [4, 7] and those calculated from the hyperfine field measured at the Co impurity [8] can be taken. The latter gives $\mu_i = 1{,}7\ \mu_B$, the former $\mu_i = 2{,}1\ \mu_B$. The concentration dependence of the saturation magnetization at low impurity concentrations is $d\mu/dc = \pm 1{,}1\ \mu_B$[9]. Assuming $\mu_i = 1{,}9\ \mu_B$, /1/ gives $dH_{av}/dc = +190$ kOe, in agreement with the experimental value. The rather large CEP contribution of +120 kOe shows that the conduction electron polarization plays an important role in the hyperfine field distribution even in the case of a transitional impurity in iron.

The Campbell-Daniel-Friedel model, which gives a good description of hyperfine fields at the impurity sites [10] [6], also explains the measured average hyperfine field in Fe-Co alloys. The question of the radial distribution of the perturbation, however, needs further investigation.

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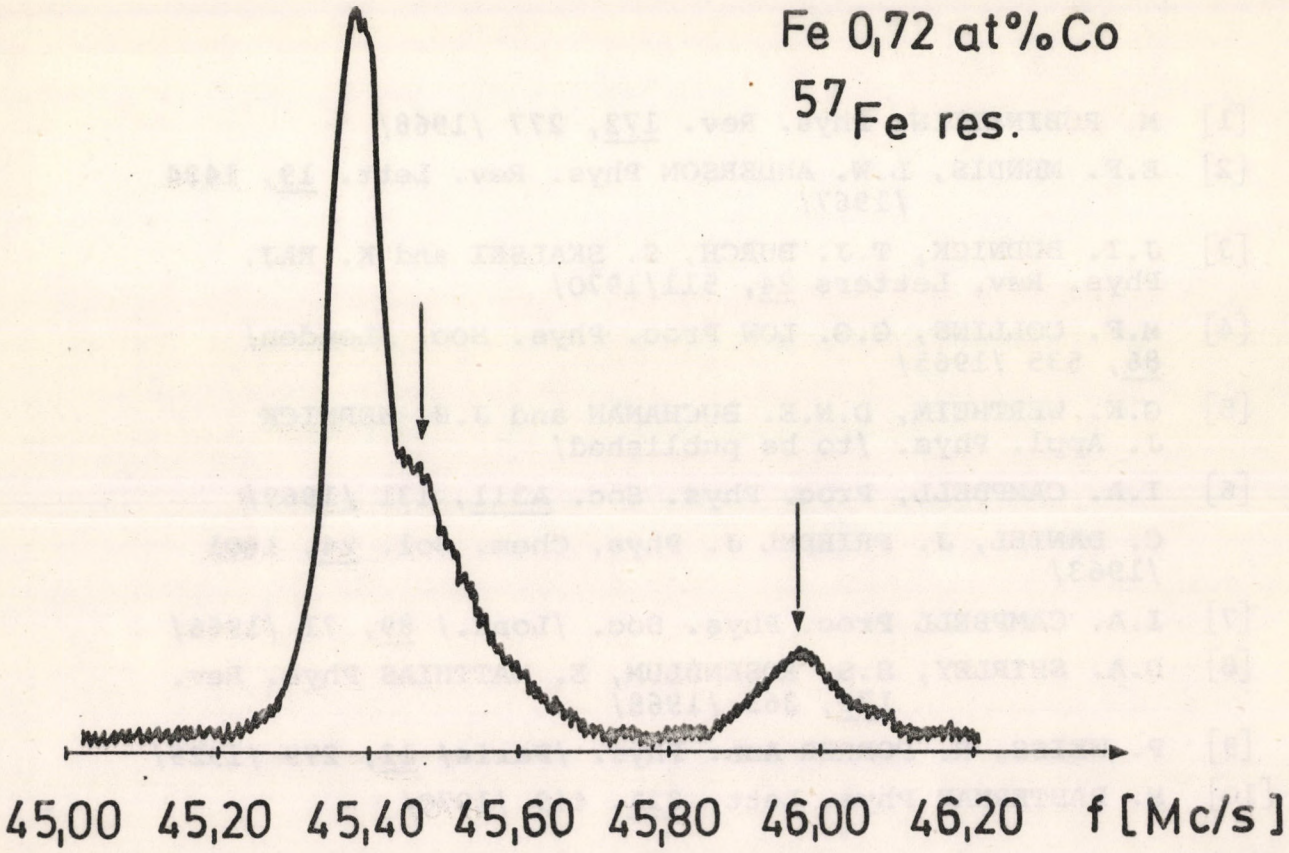

Fig. 1. ^{57}Fe cwNMR spectrum in Fe-0,72 at% Co alloy at room termperature.

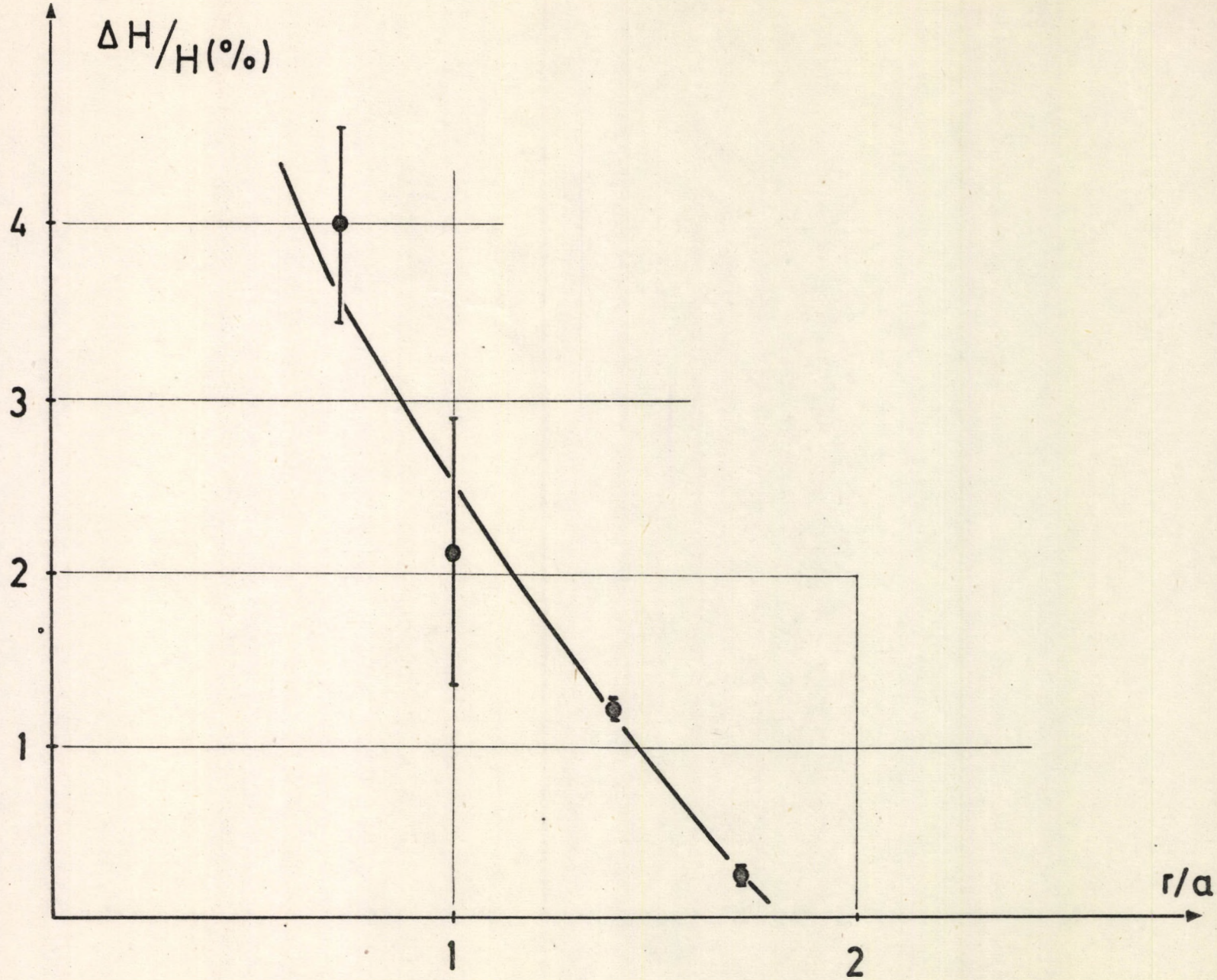

Fig. 2. Hyperfine field distribution around Co impurities in Fe-Co alloys

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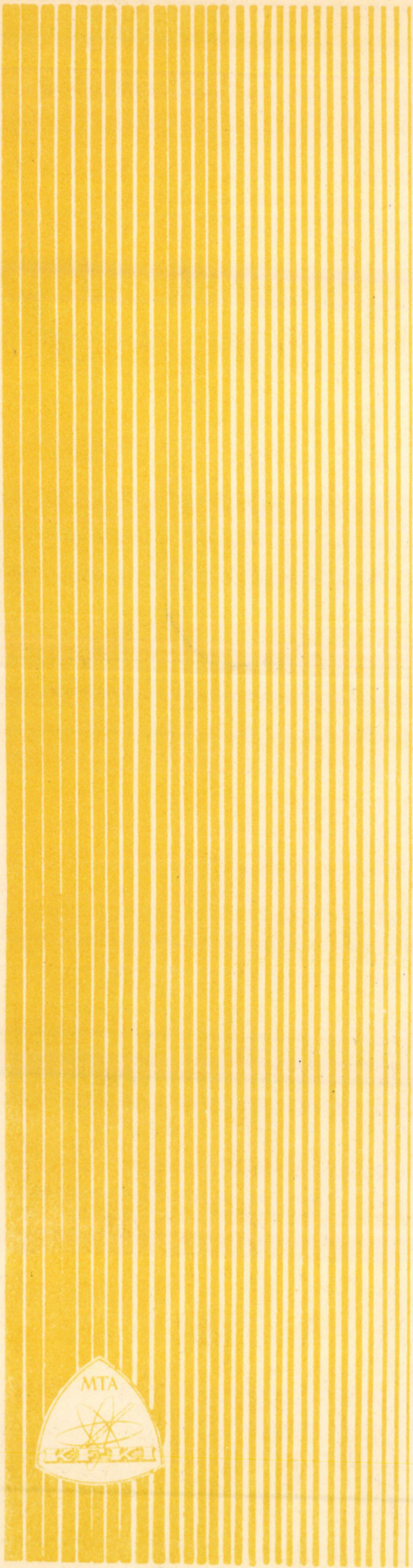

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